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SOME COMPUTATIONALLY-PREDICTED PROPERTIES
OF A GROUP OF PROPOSED ENERGETIC COMPOUNDS

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13. ABSTRACT (Maximum 200 words)

We have carried out computational analyses and predictions of certain properties for a group of proposed energetic target compounds. The properties reported are: Heat of formation, 298 K, gaseous; heat of sublimation, 298 K; heat of formation, 298 K, solid; heat of fusion at melting point; heat of vaporization at boiling point; density, liquid; boiling point; impact sensitivity. Of the molecules considered, 1,3,5,7-tetranitro-2,4,6,8-tetraazacubane is particularly promising as a potential energetic compound.

14. SUBJECT TERMS

heat of formation, heat of sublimation, heat of fusion, heat of vaporization, liquid density, boiling point, impact sensitivity

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We have carried out computational analyses and predictions of certain properties for a group of structures that were proposed by H. L. Ammon (University of Maryland) as potential energetic target compounds. The properties that will be reported, and the references describing the computational methods used, are as follows:

Heat of formation, 298 K, gaseous: ΔH_f (g), reference 1.

Heat of sublimation, 298 K: ΔH_{sub}, reference 2.

Heat of formation, 298 K, solid: ΔH_f (s)

$$\Delta H_f \text{ (s)} = \Delta H_f \text{ (g)} - \Delta H_{sub}$$

Heat of fusion at melting point: ΔH_{fus} (mp), reference 3.

Heat of vaporization at boiling point: ΔH_{vap} (bp), reference 4.

Density, liquid; reference 3.

Boiling point; reference 5.

Sensitivity: Estimates of impact sensitivity are given for four structures and shock sensitivity for two; the references will be cited individually. To put these values in perspective, the measured sensitivities of RDX on these scales are: impact sensitivity = h_{50} = 26 cm; shock sensitivity = 2.5 inches. We do not presently have a procedure for estimating the sensitivities of NF_2 derivatives.

Comments:
 (1)   We do not give predictions of solid densities, because this has already been done by H. L. Ammon.

 (2) ΔH_{sub} (298 K) $\neq \Delta H_{fus}$ (mp) + ΔH_{vap} (bp) due to the differences in temperatures.

 (3)   We do not presently have a procedure for predicting melting points; this is in progress.

Recommendation:
   We have suggested earlier, on the basis of computational studies, that the 1,3,5,7-tetranitro-2,4,6,8-tetraazacubane **5** merits particular consideration as a potential energetic compound [J. S. Murray, J. M. Seminario and P. Politzer, Struct. Chem. **2**, 153 (1991)]. Further support for this recommendation is provided by the present predictions for (a) ΔH_f (solid) in calories/gram, which is what is relevant for energetic performance, (b) sensitivity, and (c) solid state density (2.138 g/cm^3, as calculated by H. L. Ammon).

References:

1. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, J. Comp. Chem., 16, 654 (1995).

2. M. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.

3. J. S. Murray, T. Brinck and P. Politzer, Chem. Phys. 204, 289 (1996).

4. J. S. Murray and P. Politzer, in Quantitative Treatments Of Solute/Solvent Interactions, P. Politzer and J. S. Murray, eds., Vol 1, Elsevier, Amsterdam, 1994, Chapter 8.

5. J. S. Murray, P. Lane, T. Brinck, K. Paulsen, M. E. Grice and P. Politzer, J. Phys. Chem. 97, 9369 (1993).

6. J. S. Murray, P. Lane and P. Politzer, Mol. Phys. 85, 1 (1995).

7. J. S. Murray and M. E. Grice, code PREDICTOR, U. S. Army Armament, Research, Development and Engineering Center, Dover, NJ.

8. P. Lane, unpublished work.

1
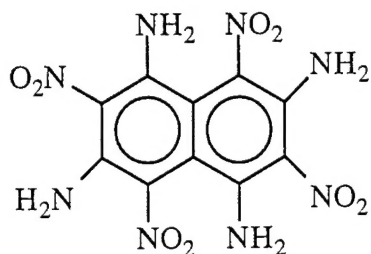
ΔH_f (g) = 17 kcal/mole

ΔH_f (s) = −24 kcal/mole = −65 cal/g

ΔH_{sub} (298 K) = 41 kcal/mole

ΔH_{fus} (mp) = 7 kcal/mole

ΔH_{vap} (bp) = 18 kcal/mole

Density (liquid) = 1.82 g/cm^3

Boiling pt. = 576 °C

Impact sensitivity: $h_{50} \gg 320$ cm (ref. 6)

2
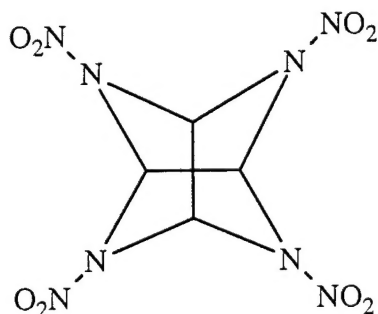
ΔH_f (g) = 114 kcal/mole

ΔH_f (s) = 84 kcal/mole = 288 cal/g

ΔH_{sub} (298 K) = 30 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 15 kcal/mole

Density (liquid) = 1.82 g/cm^3

Boiling pt. = 425 °C

Impact sensitivity: h_{50} = 42 cm (ref. 7)
h_{50} = 37 cm (ref. 8)

Shock sensitivity: 2.4 inches (ref. 7)

3
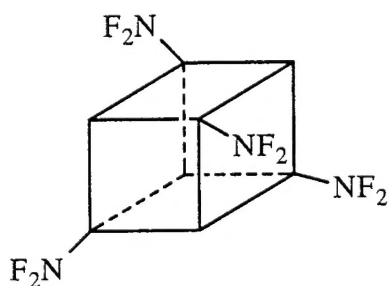
ΔH_f (g) = 73 kcal/mole

ΔH_f (s) = 43 kcal/mole = 141 cal/g

ΔH_{sub} (298 K) = 30 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 15 kcal/mole

Density (liquid) = 1.76 g/cm^3

Boiling pt. = 415 °C

4
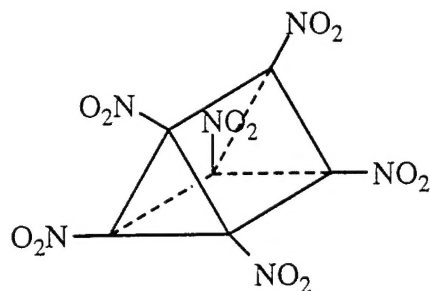
ΔH_f (g) = 179 kcal/mole

ΔH_f (s) = 144 kcal/mole = 414 cal/g

ΔH_{sub} (298 K) = 35 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 16 kcal/mole

Density (liquid) = 1.89 g/cm^3

Boiling pt. = 487 °C

Impact sensitivity: h_{50} = 6 cm (ref. 7)

Shock sensitivity = 2.7 inches (ref. 7)

5
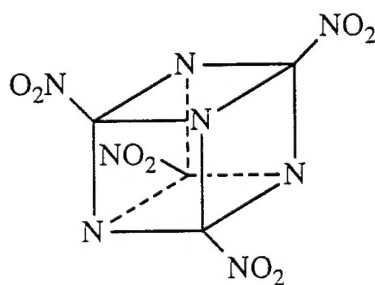
ΔH_f (g) = 216 kcal/mole

ΔH_f (s) = 189 kcal/mole = 656 cal/g

ΔH_{sub} (298 K) = 28 kcal/mole

ΔH_{fus} (mp) = 4 kcal/mole

ΔH_{vap} (bp) = 14 kcal/mole

Density (liquid) = 1.83 g/cm^3

Boiling pt. = 389 °C

Impact sensitivity: h_{50} < 160 cm (ref. 6)

6
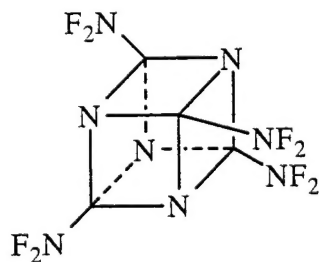
ΔH_f (g) = 141 kcal/mole

ΔH_f (s) = 114 kcal/mole = 365 cal/g

ΔH_{sub} (298 K) = 27 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 14 kcal/mole

Density (liquid) = 1.88 g/cm^3

Boiling pt. = 381 °C